SELF-CONSISTENT AB INITIO CALCULATIONS FOR PHOTOIONIZATION AND RECOMBINATION

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Most astrophysical plasmas entail a balance between ionization and recombination. We present new results from a unified method for self-consistent and ab initio calculations for the inverse processes of photoionization and (e + ion) recombination. The treatment for (e + ion) recombination subsumes the non-resonant radiative recombination and the resonant dielectronic recombination processes in a unified scheme (S.N. Nahar and A.K. Pradhan, Phys. Rev. A 49, 1816 (1994);H.L. Zhang, S.N. Nahar, and A.K. Pradhan, J.Phys.B, 32,1459 (1999)). Calculations are carried out using the R-matrix method in the close coupling approximation using an identical wavefunction expansion for both processes to ensure self-consistency.

The results for photoionization and recombination cross sections may also be compared with state-of-the-art experiments on synchrotron radiation sources for photoionization, and on heavy ion storage rings for recombination. The new experiments display heretofore unprecedented detail in terms of resonances and background cross sections and thereby calibrate the theoretical data precisely. We find a level of agreement between theory and experiment at about 10 % for not only the ground state but also the metastable states. The recent experiments therefore verify the estimated accuracy of the vast amount of photoionization data computed under the OP, IP and related works. features. Present work also reports photoionization cross sections including relativistic effects in the Breit-Pauli R-matrix (BPRM) approximation. Detailed features in the calculated cross sections exhibit the missing resonances due to fine structure.

Self-consistent datasets for photoionization and recombination have so far been computed for approximately 45 atoms and ions. These are being reported in a continuing series of publications in Astrophysical J. Supplements (e.g. references below). These data will also be available from the electronic database TIPTOPBASE (http://heasarc.gsfc.nasa.gov)

References:

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